Modelling of the refrigerant distribution in a critically charged propane heat pump cycle for performance evaluation

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Modelling of the refrigerant distribution in a critically charged propane heat pump cycle for performance evaluation

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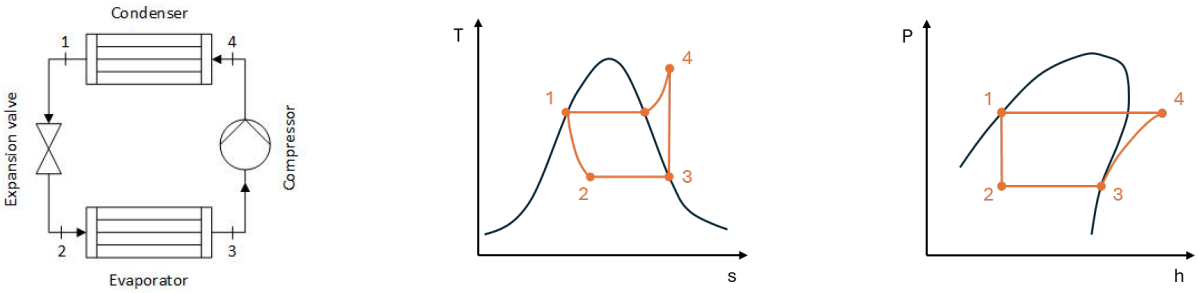
Abstract. The investigation of heat pumps employing natural refrigerants as working fluids has gained substantial momentum, driven by increasingly stringent regulations addressing the global warming potential (GWP) and ozone depletion potential (ODP) of refrigerants. Propane (R290) stands out as an attractive option due to its low GWP and zero ODP. However, a major drawback of propane lies in its flammability. When using propane as working fluid, it will therefore be necessary to limit the total refrigerant charge within the system, without compromising on the heat pump performance. This study endeavors to address this challenge by developing a model of the refrigerant charge distribution in a critically charged heat pump system consisting of an evaporator, a compressor, a condenser, and an expansion valve. In the model, the charge distribution in the two heat exchangers is modelled in detail using a suitable void fraction correlation. For the compressor and expansion valve, a simplified model is employed, in which no refrigerant charge is calculated. Using an iterative procedure, the model can then be used to determine the coefficient of performance (COP), evaporator- and condenser pressure for a heat pump with an established total charge and heat capacity. The influence of different design and operation parameters, such as the degrees of subcooling and superheat, the volume ratio of the evaporator and the condenser, etc., can be assessed.



(a) Components **(b)** Ts-diagram **(c)** Ph-diagram

Figure 1. Heat pump cycle

1. Introduction

It is widely known that the heat pump technology currently provides the best perspective for renewable heating - both residential and industrial - within the transition towards a more sustainable world. Those heat pump systems have an efficiency (defined as the ratio of useful output power to required input power) which is between three and five times higher than conventional gas boilers [1]. An important note is, however, that this heat pump technology is only as environmentally friendly as the production method of the electricity used. Another important factor for the environment is the working fluid used in the heat pump system. Driven by the increasingly strict regulations on the global warming potential (GWP) and ozone depletion potential (ODP), the implementation of natural refrigerants is more and more investigated. One of the most suitable natural refrigerants is propane (R290) due to its favourable thermodynamic properties, low cost and wide availability. The main disadvantage of propane, however, is its flammability. For safety reasons, the amount of charge within a propane heat pump should therefore be limited, ideally without compromising on performance. Various studies [2, 3, 4] have been performed on the charge reduction for a (propane) heat pump system with a fixed geometry or several possible geometries. However, in this study, the aim is to develop a model to evaluate the influence of design choices on the charge distribution from a more fundamental point of view. In this study, the considered cycle consists only of the four fundamental heat pump components: an expansion valve, an evaporator, a compressor and a condenser. This is represented schematically in figure 1a. In figures 1b and 1c, the corresponding ideal Ts- and Ph-diagram are given. Often, buffer vessels in the form of a liquid receiver after the condenser or an accumulator after the evaporator are present, but since they contain unwanted additional charge, they are disregarded in this study. Furthermore, in reality, state 1 and 3 are usually not saturated, but respectively subcooled liquid and superheated vapor states. The subcooling of state 1 makes sure the full potential of the condenser is used, while the superheating of state 3 avoids any liquid refrigerant entering in the compressor. Another non-ideality of a real system is that the compression is not isentropic, like in figure 1b, but the losses depend on the isentropic efficiency of the compressor.

The goal of this study is to develop a heat pump model and use it to investigate the effect of the refrigerant charge in the system on its operating point and consequent coefficient of performance (COP). The latter is calculated as the ratio of the heat delivered by the condenser to the power required by the compressor. The heat pump model consists of a finite volume heat exchanger model for the condenser and evaporator and a simplified model for the compressor and expansion valve. The reason is that the vast majority of the charge is situated within the heat exchangers [4], more specifically in the condenser. Furthermore, a change of charge at the same operating point is expected to mostly affect the charge in the heat exchangers, such that a simplified model suffices for the other two components, which are assumed not to contain any charge. The models, iteration procedures and results are discussed in the coming sections.

2. Heat exchanger model

To model the charge distribution of the heat exchangers, a finite volume method is used in which the transition between the different phases is implemented. Compared to a moving boundary method separating the phases, the finite volume method is computationally more expensive, but the implementation is more straightforward, as the same model can be used for both heat exhangers, and a more accurate distribution of charge can be obtained. The pressure drop is disregarded in the current version of the model to reduce the computational cost.

2.1. Single phase flow

Disregarding the pressure drop, the single-phase flow model is fairly simple: all transferred heat is directly translated in an enthalpy (h) change of the flow as follows:

$$q_i = U \cdot (T_{surrounding} - T_i) \tag{1}$$

$$h_{i+1} = h_i + q_i \cdot P \cdot \delta z / \dot{m} \tag{2}$$

with q the heat flux, P the perimeter (inner tube circumference), δz the length of one discretization step, and $\dot{m}$ the mass flow rate. It is chosen to apply a fixed heat transfer coefficient (U) per region of the two heat exchangers. In total, six heat transfer coefficients are defined: $U_{evap,l}, U_{evap,tp}, U_{evap,v}, U_{cond,v}, U_{cond,tp}, U_{cond,l}$. The values of the heat transfer coefficients can easily be changed and in a possible next version of the model, correlations can be used to determine the convective heat transfer coefficients. From the values of both enthalpy and pressure, the state at each point is fixed. Using the volume of one cell and the density of the fluid inside that cell, the mass of the fluid per cell can be calculated.

2.2. Two-phase flow

Within the two-phase zone, the calculations are somewhat more elaborate. At the edge of each cell, the following properties are calculated for both the vapor and the liquid phase: velocity (u), mass flow rate ($\dot{m}$) and area (A). Furthermore, for the two phases together, the properties considered are: void fraction (α), vapor quality (x), enthalpy (h), and temperature (T). The inlet state and mass flow rate are considered known. The system of equations consists of the conservation of mass and energy and derived continuity equations:

$$\frac{\partial \dot{m}_v}{\partial z} + \frac{\partial \dot{m}_l}{\partial z} = 0 \tag{3}$$

$$\frac{\partial \dot{m}_v}{\partial z} = A_v \cdot \rho_v \cdot \frac{\partial u_v}{\partial z} + u_v \cdot \rho_v \cdot \frac{\partial A_v}{\partial z} \tag{4}$$

$$\frac{\partial \dot{m}_l}{\partial z} = A_l \cdot \rho_l \cdot \frac{\partial u_l}{\partial z} + u_l \cdot \rho_l \cdot \frac{\partial A_l}{\partial z} \tag{5}$$

$$\frac{\partial A_v}{\partial z} + \frac{\partial A_l}{\partial z} = 0 \tag{6}$$

$$\frac{\partial A_v}{\partial z} = A \cdot \frac{\partial \alpha}{\partial z} \tag{7}$$

$$h_v \cdot \frac{\partial \dot{m}_v}{\partial z} + h_l \cdot \frac{\partial \dot{m}_l}{\partial z} = q \cdot P \tag{8}$$

$\frac{\partial \alpha}{\partial z}$ is obtained using a void fraction correlation via the $fluids$ library [6] in Python to calculate the updated version of α. q is found using equation 1. Solving the complete system of equations gives the values of all of the partial derivatives to z. From the calculated partial derivatives, $\frac{\partial h}{\partial z}$, $\frac{\partial T}{\partial z}$ and $\frac{\partial x}{\partial z}$ can be obtained. The mass of fluid in each cell can now be obtained because the void fraction, cell volume, and density of liquid and vapor phase are known.

2.3. Iteration scheme

Since multiple phase zones are present within both the condenser and the subcooler, a scheme is followed in the model on when to transition between the different phases. The followed procedure is visualised in figure 2. The treshold values that are used for the enthalpy are those of saturated vapor and liquid. The equations described in sections 2.1 and 2.2 are applied respectively in the sigle phase and two-phase zones.

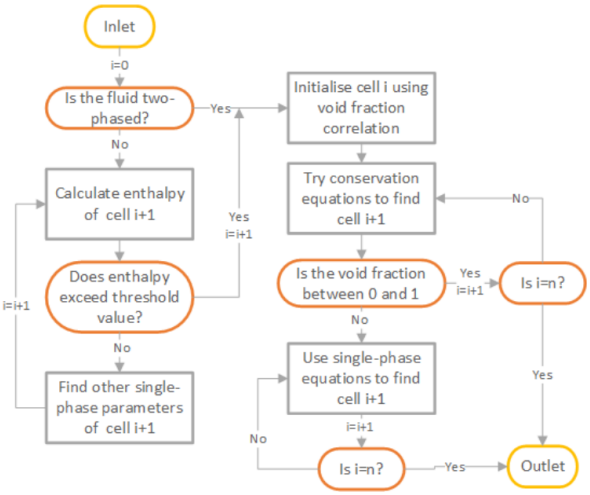


Figure 2. Heat exchanger iteration

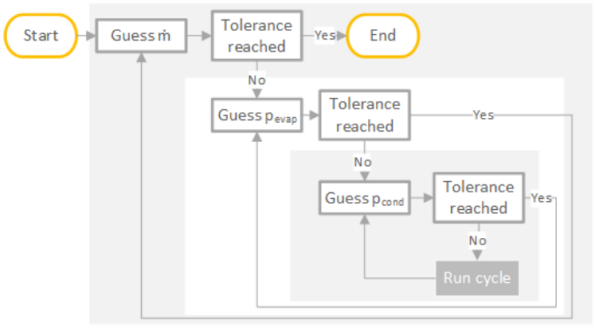


Figure 3. Heat pump iteration scheme

3. Heat pump model

As mentioned before, a chargeless model for the expansion valve and the compressor are used. The expansion valve is modelled as being an isenthalpic process. When the condenser pressure ($p_1 = p_4$) and subcooling after the condenser ($T_{sat}(p_1) - T_1$) are known, the state before the expansion valve is fixed. The state after the expansion valve is then found using the evaporator pressure ($p_2 = p_3$) and the assumption of an isenthalpic valve: $h_2 = h_1$.

To determine state 4, the compressor is modelled using an isentropic efficiency (η_c), which is, assuming an adiabatic process, defined as the ratio of enthalpy difference over the compressor in case of isentropic compression ($h_{4s} - h_3$) to the real compression ($h_4 - h_3$).

For given values of the compressor efficiency, geometry of the heat exchangers, surrounding temperatures of the condenser and evaporator, heat transfer coeffcients, subcooling after the condenser, mass flow rate, condenser- and evaporator pressures, all states in the heat pump cycle can be calculated. However, when calculating the cycle from state 1 on and ending in state 1', there will be an enthalpy difference if the above mentioned values are not chosen correctly. Furthermore, the goal of the model is to find the performance when the heat pump is charged with an established mass of refrigerant and capacity. To be able to meet those three constraints (closed cycle, total charge and capacity), the mass flow rate, evaporator- and condenser pressure are variable and will be changed such that the requirements are fulfilled. The procedure of how the mass flow rate, evaporator- and condenser pressure are then found, is illustrated in figure 3. In the inner loop, the condenser pressure is changed until the cycle is closed, which means the enthalpy difference between state 1 and 1' is below the treshold value. In the middle loop, the evaporator pressure is changed, such that the total charge is equal to the desired value. The outer loop makes sure the capacity is the desired one by changing the mass flow rate of the working fluid. The secant method is used to find a solution in each loop.

4. Results

For the simulations presented in this work, the values of the different parameters can be found in table 1. These parameters are easily changed, such that the model can be used for a wide diversity of heat pumps. However, to validate the influence of two parameters, more specifically total charge and ratio of heat exchanger volume ($\beta = V_{cond}/V_{evap}$), on the performance and operating point, the values in table 1 were fixed for all simulations.

Figure 4 shows the results of the simulations for three different β-values and different charges.

General		**Evaporator**		**Condenser**	
η_c	0.7	Number of tubes	20	Number of tubes	20
Subcooling	5°C	Length of tubes	6m	Inner diameter	7mm
Heat source T	-7°C	Inner diameter	7mm	U vapor zone	200W/m^{2}K
Heat sink T	20°C	U vap/liq zone	100W/m^{2}K	U liquid zone	500W/m^{2}K
Heat capacity	10kW	U two-phase zone	1000W/m^{2}K	U two-phase zone	2000W/m^{2}K

Table 1. Parameters heat pump simulations

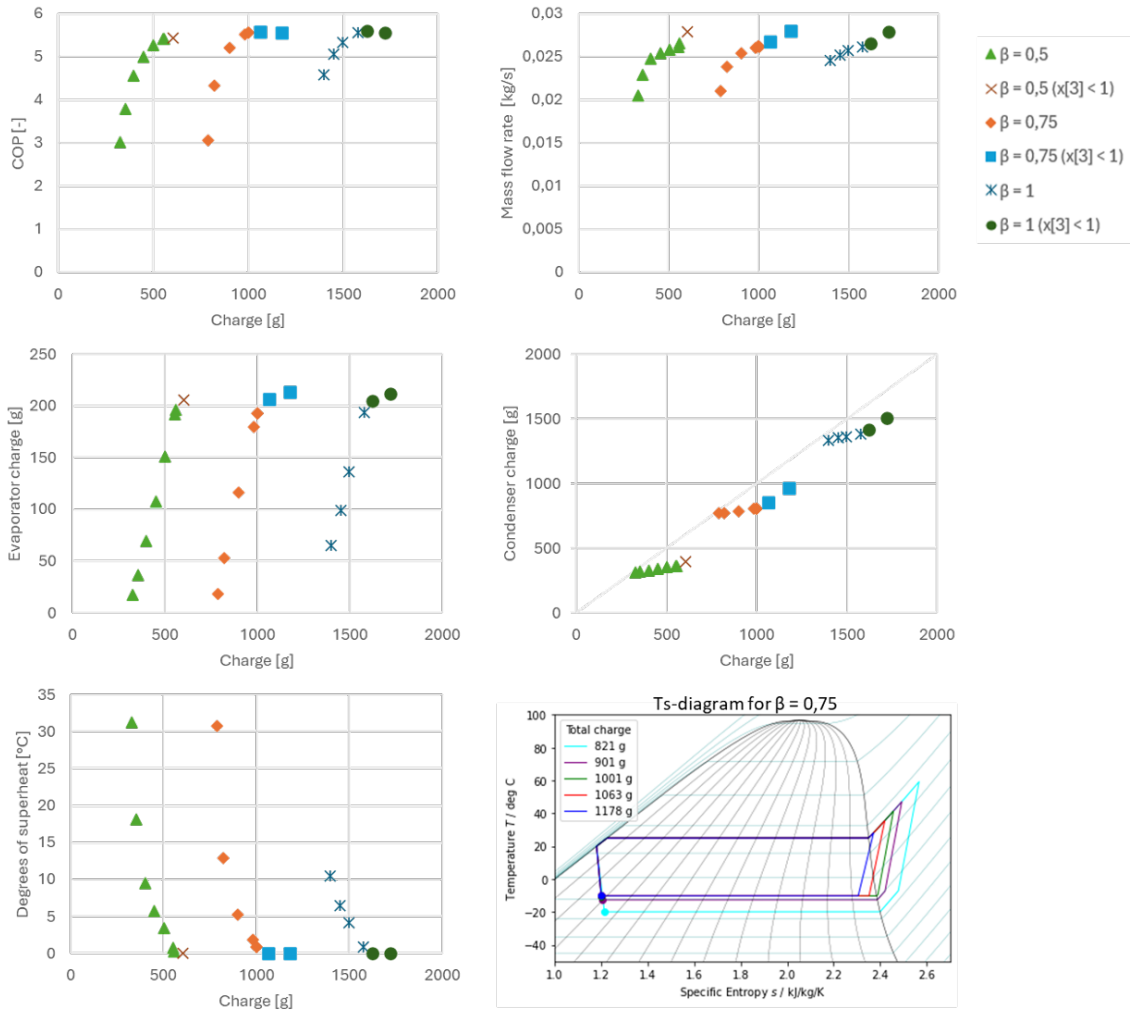


Figure 4. Effect of charge on COP, mass flow rate, evaporator- and condenser charge, and degrees of superheat

For each β-value, only a limited set of charges is shown. For lower charges, the degree of superheat quickly becomes very high, resulting in supercritical temperatures, and the COP decreases drastically. With increasing values of the charge, this superheat decreases until it reaches zero. A further increase in total charge results in a two-phase flow at the outlet of the evaporator, causing wet suction at the compressor. Some simulations where this is the case are shown ($x[3] < 1$) to illustrate the effect on the cycle.

For a specific β-value, the COP increases with increasing total charge until the point of a saturated vapor outlet of the evaporator. Furthermore, a higher total charge causes an increase in mass flow rate. When increasing the total charge, one could expect the subcooling to increase, but in the simulations presentedthe subcooling is fixed. So, a significant share of the extra mass is located in the evaporator as liquid and a smaller share as vapor in the evaporator, causing a higher evaporator pressure. This can be seen on the Ts-diagram for $\beta = 0.75$. The higher evaporator pressure corresponds to a higher saturation temperature of the propane in the evaporator and thus a lower temperature difference between propane and heat source. So, a higher mass flow rate is needed such that sufficient heat is transferred to the working fluid in the evaporator to deliver the imposed condenser capacity, causing a lower (and eventually zero) superheat. The trends of COP and charge distribution agree with previous studies [2, 3].

An increase in β-value corresponds to a larger condenser volume, since the evaporator geometry is fixed and β is the volume ratio of condenser to evaporator. A larger β-value goes together with a higher total charge under the current boundary conditions of fixed condenser capacity and subcooling. The graph showing the condenser charge reveals this additional charge is mainly stored in the condenser. Further analysis of the results showed this extra condenser charge is mainly in liquid state. From the performed simulations, the maximum COP value seems to increase with β, but from $\beta = 0.75$ to $\beta = 1$ the increase is very small. The reason is that the pinch point temperature difference in the condenser almost does not change anymore.

5. Conclusion

In this work, a model is presented that was built to understand the charge distribution in a critically charged propane heat pump system and to assess the effect of the total charge on the COP and operating point. The two heat exchangers were modelled using a finite volume approach, while the expansion valve and compressor were modelled not to contain any charge. The simulations using a fixed condenser capacity and subcooling showed an increase in COP with increasing total charge until the point of no superheat. A lower total charge, on the other hand, caused a large degree of superheat and decreased COP. The COP also increased with a larger condenser volume, and consequently more charge. However, increasing the condenser volume beyond a $\beta = V_{cond}/V_{evap} = 0.75$ has negligible impact, as the temperature difference between the refrigerant and the secondary fluid has already reached a value of less than 0.1 °C. Possibilities for extending the model are the modelling of the compressor charge, adding pressure drop in the heat exchanger models, and fixing the degrees of superheat instead of the subcooling. Another interesting further approach would be to change the boundary conditions for a certain fixed design such that the off-design performance can be evaluated.

Acknowledgements

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References

[1] International Energy Agency 2022 The Future of Heat Pumps.(`www.iea.org`)
[2] Methler T, Dankwerth C, Joos L, Fugmann H, Morawietz K and Schnabel L 2022 Experimental Analysis of Various Refrigerant Circuit Component Combinations for Low Charge Propane Heat Pumps *15th IIR Gustav Lorentzen Conf. on Natural Refrigerants: Natural Refrigerant Solutions for Warm Climate Countries*
[3] Fernando P, Palm B, Lundqvist P and Granryd E 2004 Propane Heat Pump with Low Refrigerant Charge: Design and Laboratory Tests *Int. J. of Refr.* **27** 761-773
[4] Corberán J M, Martínez I O and Gonzálvez J 2008 Modelling of Refrigerant Charge to Investigate Heat Pump Performance with Alternative Refrigerants *Int. J. of Refr.* **31** 716-726
[5] Deblaere T, Lecompte S and De Paepe M 2022 Modelling of Refrigerant Charge to Investigate Heat Pump Performance with Alternative Refrigerants *Master thesis Electromechanical Engineering, Ghent University*
[6] Bell C and contributors 2016-2023 fluids: Fluid dynamics component of Chemical Engineering Design Library (ChEDL) (`https://github.com/CalebBell/fluids`)